International Journal of Mathematics and Computer Applications Research (IJMCAR)
ISSN(P): 2249-6955; ISSN(E): 2249-8060
Vol. 4, Issue 2, Apr 2014, 11-18

THE PROBLEM OF D-OPTIMALITY IN SOME EXPERIMENTAL DESIGNS

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ABSTRACT

We consider we problem of determining of D-optimal experimental designs. During many possible experimental plans we consider designs called chemical balance weighing designs that are described by the linear model. We study the problem of determining optimal design under assumption that the measurement errors are equal correlated.

KEYWORDS: Chemical Balance Weighing Design, D-Optimal Design, Experimental Design

Classification AMS 2010: 62K05, 62K10

1. INTRODUCTION

The planning of experiments is very important part of mathematical statistics. Among many conditions determining best experimental plan, very significant is to fix the optimality criterion. The choice of optimality criterion influences on the properties of determined estimators. In many papers, some problems related to the determining of the optimality criterion and the consequences of this choice are considered (See Pukelsheim, 1993). For the most part, the optimality criteria there are functions of the design matrix. In determining the best experimental plan, we have to remember about the experimental model. In present paper we consider chemical balance weighing design. Such designs can be applied in economy, agriculture, optics. Chemical balance weighing design there is the model of experimental design that permits to determining unknown measurements of p objects if we will take them n times in different combinations to measure. The results of n measurement operations of p objects will fit into the linear model $\mathbf{y} = \mathbf{X}\mathbf{w} + \mathbf{e}$, where $\mathbf{y}$ is the $n \times 1$ random vector of observed weights, $\mathbf{X} \in \mathbf{\Phi}_{n\times p,m}(-1, 0, 1)$, $\mathbf{\Phi}_{n\times p,m}(-1, 0, 1)$ denotes the class of $n \times p$ matrices $\mathbf{X} = (x_{ij})$, $i = 1,2,\dots,n$, $j = 1,2,\dots,p$, of known elements equal to -1, 1 or 0 according as in the ith weighing operation the jth object is placed on the right pan, left pan or not and $m = \max\{m_1, m_2, \dots, m_p\}$, where m_j, $j = 1,2,\dots,p$, represents the number of elements equal to -1 and 1 in jth column of $\mathbf{X}$, $\mathbf{w}$ is a $p \times 1$ vector representing unknown weights of objects and $\mathbf{e}$ is an $n \times 1$ random vector of errors. Additionally, we assume that there are not systematic errors, i.e. $\mathrm{E}(\mathbf{e}) = \mathbf{0}_n$ and $\mathrm{Var}(\mathbf{e}) = \sigma^2\mathbf{G}$, where σ^2 is the constant variance errors, $\mathbf{G}$ is $n \times n$ known positive definite matrix of the form

$$\mathbf{G} = g\left[(1-\rho)\mathbf{I}_n + \rho\mathbf{1}_n\mathbf{1}_n^{'}\right], \quad g > 0, \frac{-1}{n-1} < \rho < 1 \tag{1}$$

The form of the matrix $\sigma^2\mathbf{G}$ means that the measurement errors are correlated. Let note, $\mathbf{G}^{-1} = \frac{1}{g(1-\rho)}\left[\mathbf{I}_n - \frac{\rho}{1+\rho(n-1)}\mathbf{1}_n\mathbf{1}_n^{'}\right]$. For estimation $\mathbf{w}$ we use the normal equations $\mathbf{X}^{'}\mathbf{G}^{-1}\mathbf{X}\mathbf{w} = \mathbf{X}^{'}\mathbf{G}^{-1}\mathbf{y}$. Any chemical balance weighing design is singular or nonsingular depending on whether $\mathbf{X}^{'}\mathbf{G}^{-1}\mathbf{X}$ is singular or nonsingular, respectively. Since $\mathbf{G}$ is known positive definite matrix then $\mathbf{X}^{'}\mathbf{G}^{-1}\mathbf{X}$ is nonsingular if and only if $\mathbf{X}$ is of full column rank. However, if $\mathbf{X}^{'}\mathbf{G}^{-1}\mathbf{X}$ is nonsingular then the generalized least squares estimator of $\mathbf{w}$ is given by $\hat{\mathbf{w}} = \left(\mathbf{X}^{'}\mathbf{G}^{-1}\mathbf{X}\right)^{-1}\mathbf{X}^{'}\mathbf{G}^{-1}\mathbf{y}$ and $\mathrm{Var}(\hat{\mathbf{w}}) = \sigma^2\left(\mathbf{X}^{'}\mathbf{G}^{-1}\mathbf{X}\right)^{-1}$. The matrix $\mathbf{M} = \mathbf{X}^{'}\mathbf{G}^{-1}\mathbf{X}$ is called the information matrix of the design $\mathbf{X}$.

In many problems concerning experimental designs the D-optimal designs are considered. In the case of chemical balance weighing designs, the design $\mathbf{X}_d$ is D-optimal in the class of the design matrices $\mathbf{\Psi} \subset \mathbf{\Phi}_{n\times p,m}(-1, 0, 1)$ if $\det\left(\mathbf{X}_d^{'}\mathbf{G}^{-1}\mathbf{X}_d\right) = \max\{\det(\mathbf{M}) : \mathbf{X} \in \mathbf{\Psi}\}$. It is known that $\det(\mathbf{M})$ is maximal if and only if $\det\left(\mathbf{M}^{-1}\right)$ is minimal. The concept of D-optimality was considered in the books of Raghavarao (1971), Banerjee (1975), Shah and Sinha (1989). In the paper Jacroux et al. (1983) the problems related to the D-optimality were presented for the case $\mathbf{G} = \mathbf{I}_n$. In Masaro and Wong (2008), Katulska and Smaga (2013), D-optimal weighing designs $\mathbf{X} \in \mathbf{\Lambda}_{n\times p}(-1, 1)$, where $\mathbf{\Lambda}_{n\times p}(-1, 1)$ is the set of all $n \times p$ matrices with elements -1 or 1, only, are considered.

In this paper, we present new results concerned D-optimal chemical balance weighing designs that are the generalization of given in Katulska and Smaga (2013) ones. We assume that the random errors are equally correlated and they have equal variances. We give lower bound for the determinant of the inverse of information matrix. Also we give the examples of the D-optimal chemical balance weighing design for which the determinant of the inverse of information matrix attains the lower bound.

2. D-OPTIMAL DESIGN

Let $\mathbf{X} = \left[\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_p\right] \in \mathbf{\Phi}_{n\times p,m}(-1, 0, 1)$. From Section 1.c.1(ii) (b), Rao (1973) we have

Lemma 2.1: Let $\mathbf{G}$ be as in (1). For diagonal elements of the inverse of information matrix the following inequality holds

$$\mathbf{M}_{jj}^{-1} = \left(\mathbf{x}_j^{'}\mathbf{G}^{-1}\mathbf{x}_j\right)^{-1} \geq \frac{g(1-\rho)}{\mathbf{x}_j^{'}\mathbf{x}_j - \frac{\mathbf{x}_j^{'}\mathbf{1}_n\mathbf{1}_n^{'}\mathbf{x}_j\rho}{1+\rho(n-1)}}. \tag{2}$$

Now, we prove the inequality which gives the lower bound for the determinant of the inverse of information matrix.

Theorem 2.1: Let $\mathbf{G}$ be as in (1). If $\mathbf{X} \in \mathbf{\Phi}_{n\times p,m}(-1, 0, 1)$ then

$$\det\left(\mathbf{M}^{-1}\right) \geq \begin{cases} \left(\dfrac{g(1-\rho)}{m}\right)^{p} & \text{if} \quad 0 \leq \rho < 1 \\ \left(\dfrac{g(1-\rho)}{m - \dfrac{\rho(m-2u)^2}{1+\rho(n-1)}}\right)^{p} & \text{if} \quad \dfrac{-1}{n-1} < \rho < 0 \end{cases} \tag{3}$$

Where $u = \min\{u_1, u_2, \ldots, u_p\}$, u_j represents the number of elements equal to -1 in j th column of $\mathbf{X}$, $j = 1,2,\ldots,p$.

Proof: By the Hadamard's inequality it follows that

$$\det\left(\mathbf{M}^{-1}\right) \geq \prod_{j=1}^{p} \mathbf{M}_{jj}^{-1} = \prod_{j=1}^{p}\left(\mathbf{x}_j^{'}\mathbf{G}^{-1}\mathbf{x}_j\right)^{-1}. \tag{4}$$

Hence by Lemma 2.1 we obtain $\left(\mathbf{x}_j^{'}\mathbf{G}^{-1}\mathbf{x}_j\right)^{-1} \geq g(1-\rho)\left(\mathbf{x}_j^{'}\mathbf{x}_j\right)^{-1}$ taking $\mathbf{x}_j^{'}\mathbf{1}_n = 0$. The maximal value of $\mathbf{x}_j^{'}\mathbf{x}_j$ is m assuming that $\mathbf{X} \in \mathbf{\Phi}_{n\times p,m}(-1, 0, 1)$. For the case $-(n-1)^{-1} < \rho < 0$, the maximal value of denominator is attained if $\dfrac{\mathbf{x}_j^{'}\mathbf{1}_n\mathbf{1}_n^{'}\mathbf{x}_j\rho}{1+\rho(n-1)}$ is maximal, so if $\mathbf{x}_j^{'}\mathbf{1}_n\mathbf{1}_n^{'}\mathbf{x}_j = (m-2u)^2$. So, the proof is completed.

Definition 2.1: Any chemical balance weighing design $\mathbf{X} \in \mathbf{\Phi}_{n\times p,m}(-1, 0, 1)$ with the covariance matrix of errors $\sigma^2\mathbf{G}$, where $\mathbf{G}$ is given by (1), is said to be regular D-optimal if it satisfies the equality in (3), that is

$$\det\left(\mathbf{M}^{-1}\right) = \begin{cases} \left(\dfrac{g(1-\rho)}{m}\right)^{p} & \text{if} \quad 0 \leq \rho < 1 \\ \left(\dfrac{g(1-\rho)}{m - \dfrac{\rho(m-2u)^2}{1+\rho(n-1)}}\right)^{p} & \text{if} \quad \dfrac{-1}{n-1} < \rho < 0 \end{cases} \tag{5}$$

Let note, the regular D-optimal design is D-optimal, whereas the inverse sentence may not be true.

Theorem 2.2: Any chemical balance weighing $\mathbf{X} \in \mathbf{\Phi}_{n\times p,m}(-1, 0, 1)$ with the covariance matrix of errors $\sigma^2\mathbf{G}$, where $\mathbf{G}$ is given by (1), is regular D-optimal if and only if

$\mathbf{X}^{'}\mathbf{X} = m\mathbf{I}_p$ if $\rho = 0$,

$\mathbf{X}^{'}\mathbf{X} = m\mathbf{I}_p$ and $\mathbf{X}^{'}\mathbf{1}_n = \mathbf{0}_p$ if $0 < \rho < 1$,

$\mathbf{X}^{'}\mathbf{X} = m\mathbf{I}_p - \dfrac{\rho(m-2u)^2}{1+\rho(n-1)}\left(\mathbf{I}_p - \mathbf{1}_p\mathbf{1}_p^{'}\right)$ and $\mathbf{X}^{'}\mathbf{1}_n = \mathbf{z}_p$ if $\dfrac{-1}{n-1} < \rho < 0$,

Where $\mathbf{z}_p$ is $p\times 1$ vector for which the j th element is equal to $(m-2u)$ or $-(m-2u)$, $j=1,2,\ldots,p$.

Proof: Let $\mathbf{X}\in\mathbf{\Phi}_{n\times p,m}(-1,0,1)$ be the design with the covariance matrix $\sigma^2\mathbf{G}$, where $\mathbf{G}$ is given by (1).

- If $\mathbf{X}'\mathbf{X}=m\mathbf{I}_p$ then $\mathbf{x}_j'\mathbf{x}_k=0$ for $j\neq k$, $j,k=1,2,\ldots,p$. Because of this and from Lemma 2.1 it follows that if $\rho=0$ then the inverse of the information matrix is equal to $\frac{g}{m}\mathbf{I}_p$, so its determinant satisfies (5).
- If $0<\rho<1$ and $\mathbf{x}_j'\mathbf{1}_n=0$, $j=1,2,\ldots,p$, then under Lemma 2.1 we deduce that the inverse of the information matrix of the design $\mathbf{X}$ is equal to $g(1-\rho)m^{-1}\mathbf{I}_p$ and therefore the equality (5) is also true.
- If $\mathbf{X}'\mathbf{X}=m\mathbf{I}_p-\frac{\rho(m-2u)^2}{1+\rho(n-1)}\left(\mathbf{I}_p-\mathbf{1}_p\mathbf{1}_p'\right)$ and $\mathbf{X}'\mathbf{1}_n=\mathbf{z}_p$, then by Lemma 2.1 we deduce that the inverse of the information matrix of the design $\mathbf{X}$ is equal to $g(1-\rho)\left(m-\frac{\rho(m-2u)^2}{1+\rho(n-1)}\right)^{-1}\mathbf{I}_p$ and therefore the equality (5) holds.
- Thus the design $\mathbf{X}$ is regular D-optimal in many cases. Hence Theorem.

Corollary 2.1: Let $0<\rho<1$. The necessary condition for existence regular D-optimal chemical balance weighing design $\mathbf{X}\in\mathbf{\Phi}_{n\times p,m}(-1,0,1)$ with the covariance matrix of errors $\sigma^2\mathbf{G}$, where $\mathbf{G}$ is given by (1), is $m\equiv 0\,\mathrm{mod}(2)$.

3. EXAMPLES OF REGULAR D-OPTIMAL DESIGN

In order to determine regular D-optimal chemical balance weighing design $\mathbf{X}\in\mathbf{\Phi}_{n\times p,m}(-1,0,1)$ with the covariance matrix of errors $\sigma^2\mathbf{G}$, where $\mathbf{G}$ is given by (1), we have to fix regular D-optimal design in the class $\mathbf{\Phi}_{n\times p,m}(-1,0,1)$ for each ρ separately. It means for $\rho=0$, $0<\rho<1$ and for $\frac{-1}{n-1}<\rho<0$. The assignation of the design matrix that satisfies one of the conditions 1-3 from Theorem 2.2 is connected with determining the matrix with special properties. Some methods of construction of such matrices given in literature is based on the incidence matrices of some known block designs, for example balanced incomplete block designs, ternary balanced block designs, balanced bipartite block designs. In different papers there are given the algorithms nominated the best design (See Angelis et al., 2001). The aim of this paper is to give the lower bound of the determinant of the inverse of information matrix for the design and determining of the conditions under that the lower bound is satisfied. So we will give only some examples of regular D-optimal designs.

Let $\rho=0$. We consider $\mathbf{X}\in\mathbf{\Phi}_{10\times 5,8}(-1,0,1)$. We have $\mathrm{Var}(\hat{w}_j)=\frac{g}{8}\sigma^2$, $j=1,2,\ldots,5$. Regular D-optimal chemical balance weighing design in this class is given in the form

$$\mathbf{X}^{'} = \begin{bmatrix} 1 & -1 & -1 & -1 & 0 & 1 & -1 & -1 & 0 & -1 \\ 0 & 1 & -1 & -1 & -1 & -1 & 1 & -1 & -1 & 0 \\ -1 & 0 & 1 & -1 & -1 & 0 & -1 & 1 & -1 & -1 \\ -1 & -1 & 0 & 1 & -1 & -1 & 0 & -1 & 1 & -1 \\ -1 & -1 & -1 & 0 & 1 & -1 & -1 & 0 & -1 & 1 \end{bmatrix}.$$

Now, let us consider $\mathbf{X} \in \mathbf{\Phi}_{20\times 5,16}(-1,0,1)$. $\mathbf{X} = [\,\mathbf{X}_1 \;\; \mathbf{X}_2\,]^{'}$ is the regular D-optimal chemical balance weighing design for any ρ, $0 < \rho < 1$ and $\operatorname{Var}(\hat{w}_j) = \dfrac{g(1-\rho)}{16}\sigma^2$, $j = 1,2,\ldots,5$, where

$$\mathbf{X}_1 = \begin{bmatrix} 0 & -1 & 1 & 1 & 1 \\ 1 & 0 & -1 & 1 & 1 \\ 1 & 1 & 0 & -1 & 1 \\ 1 & 1 & 1 & 0 & -1 \\ -1 & 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & -1 & 1 \\ 1 & 0 & 1 & 1 & -1 \\ -1 & 1 & 0 & 1 & 1 \\ 1 & -1 & 1 & 0 & 1 \\ 1 & 1 & -1 & 1 & 0 \end{bmatrix}, \qquad \mathbf{X}_2 = \begin{bmatrix} 0 & 1 & -1 & -1 & -1 \\ -1 & 0 & 1 & -1 & -1 \\ -1 & -1 & 0 & 1 & -1 \\ -1 & -1 & -1 & 0 & 1 \\ 1 & -1 & -1 & -1 & 0 \\ 0 & -1 & -1 & 1 & -1 \\ -1 & 0 & -1 & -1 & 1 \\ 1 & -1 & 0 & -1 & -1 \\ -1 & 1 & -1 & 0 & -1 \\ -1 & -1 & 1 & -1 & 0 \end{bmatrix}.$$

For the case $\dfrac{-1}{n-1} < \rho < 0$ we consider $\mathbf{G} = g\left[\dfrac{14}{13}\mathbf{I}_{10} - \dfrac{1}{13}\mathbf{1}_{10}\mathbf{1}_{10}^{'}\right]$. So, we determine the regular D-optimal design in the class $\mathbf{X} \in \mathbf{\Phi}_{10\times 5,6}(-1,0,1)$. We obtain

$$\mathbf{X}^{'} = \begin{bmatrix} 1 & 1 & 1 & 1 & 0 & -1 & 0 & 0 & -1 & 0 \\ 1 & 0 & 0 & -1 & 1 & 1 & 1 & -1 & 0 & 0 \\ -1 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & -1 \\ 0 & -1 & 1 & 0 & 0 & 1 & -1 & 1 & 0 & 1 \\ 0 & 0 & -1 & 1 & -1 & 0 & 1 & 0 & 1 & 1 \end{bmatrix}$$

And $\operatorname{Var}(\hat{w}_j) = \dfrac{2g}{13}\sigma^2$, $j = 1,2,\ldots,5$.

4. DISCUSSIONS

We consider the regular D-optimal chemical balance weighing design in order to determine estimators of unknown measurements of objects with the smallest variance. So, let us consider $\mathbf{X} \in \mathbf{\Phi}_{n\times p,m}(-1,0,1)$ for fixed number of n, p, m. We consider parameter ρ in intervals given in Theorem 2.2. If $\rho = 0$ then $\operatorname{Var}(\hat{w}_j) = \dfrac{g}{m}\sigma^2$, if

$0<\rho<1$ then $\operatorname{Var}(\hat{w}_j)=\frac{g(1-\rho)}{m}\sigma^2$ if $\frac{-1}{n-1}<\rho<0$ then $\operatorname{Var}(\hat{w}_j)=g(1-\rho)\left(m-\frac{\rho(m-2u)^2}{1+\rho(n-1)}\right)^{-1}\sigma^2$

$j=1,2,\ldots,p$.

In the planning of each experiment according to the model of the chemical balance weighing design, as the first step we have to choice the value of correlation of errors, i.e. ρ. Let us consider any ρ_t, $0<\rho<1$, $t=1,2$, $\rho_1 \neq \rho_2$. It is worth pointing out that the design $\mathbf{X} \in \mathbf{\Phi}_{n\times p,m}(-1,0,1)$ satisfying Theorem 2.2 is regular D-optimal in the sense of attaining equality (5), for ρ_1 and ρ_2. Thus the design $\mathbf{X} \in \mathbf{\Phi}_{n\times p,m}(-1,0,1)$ is regular D-optimal for any ρ, $0<\rho<1$. Simultaneously the lower bound of variance of estimators is not the same for different numbers of ρ. According to the paper Masaro and Wong (2008) the design is robust.

The choice of the value of ρ is very important from the point of view of estimation of unknown measurements of objects. For $0<\rho<1$, greater value of ρ implies minor value of $\operatorname{Var}(\hat{w}_j)$. For $-(n-1)^{-1}<\rho<0$, minor value of ρ implies major value of $\operatorname{Var}(\hat{w}_j)$.

In the case when the regular D-optimal design doesn't exist we have to determine the design for which the determinant of the inverse of the information matrix is the closest to given in (5) one. The lowest bound given in (5) permits to check if given design is optimal or not. In such cases some problems of determining optimal designs are given in Graczyk (2011, 2012).

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